



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:28 AM GMT

PDB ID : 2FHC
Title : Crystal Structure Analysis of Klebsiella pneumoniae pullulanase complexed with maltotriose
Authors : Mikami, B.; Iwamoto, H.; Katsuya, Y.; Yoon, H.-J.; Demirkan-Sarikaya, E.; Malle, D.
Deposited on : 2005-12-23
Resolution : 1.85 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

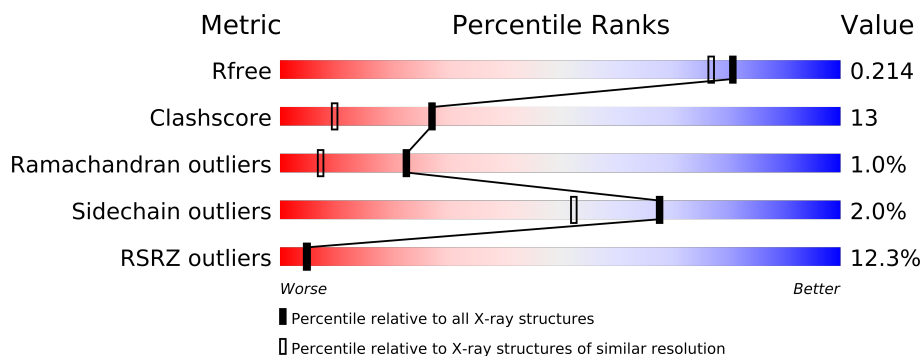
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1083	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9357 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called pullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1052	Total	C	N	O	S	0	20	0
			8142	5088	1388	1639	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	680	LEU	GLY	ENGINEERED	GB 149300
A	882	LEU	VAL	ENGINEERED	GB 149300

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			34	18	16		
2	A	3	Total	C	O	0	0
			34	18	16		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	680	LEU	GLY	ENGINEERED	GB 149300
A	882	LEU	VAL	ENGINEERED	GB 149300
A	680	LEU	GLY	ENGINEERED	GB 149300
A	882	LEU	VAL	ENGINEERED	GB 149300

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	C	O	0	0
			23	12	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	680	LEU	GLY	ENGINEERED	GB 149300
A	882	LEU	VAL	ENGINEERED	GB 149300

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Ca 5 5	0	0

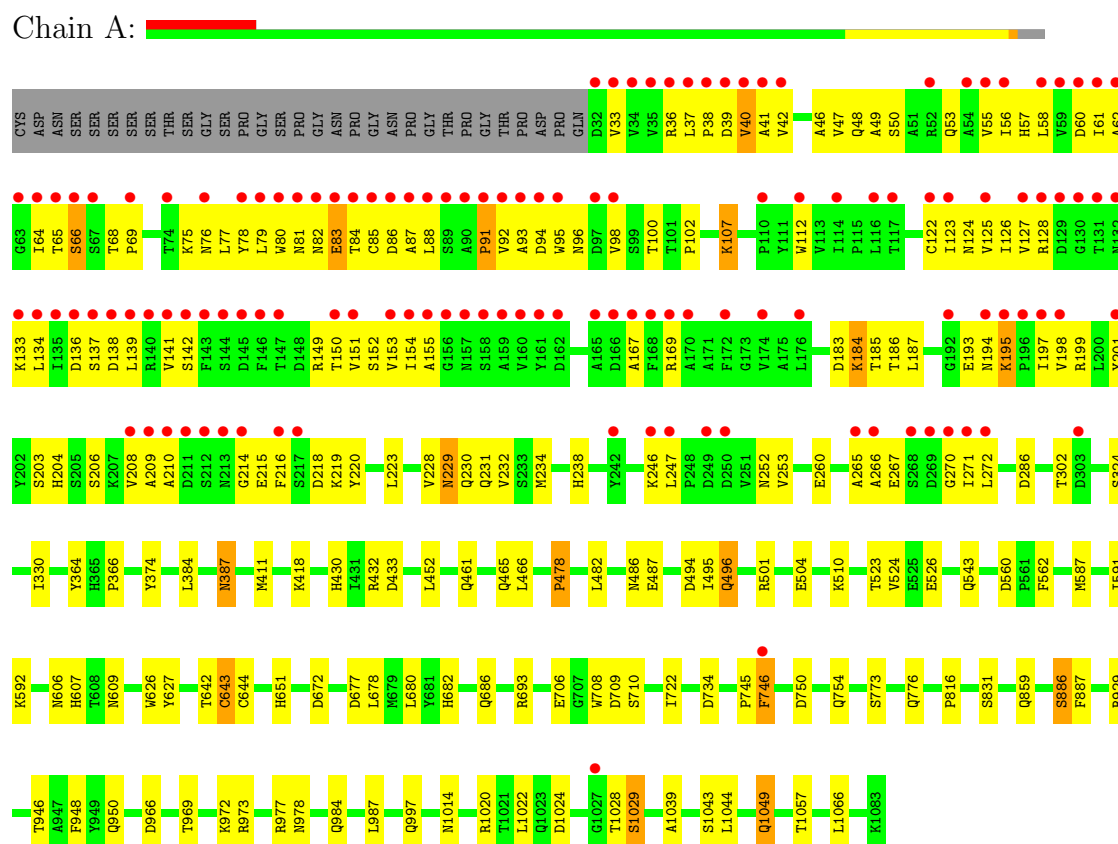
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1119	Total O 1119 1119	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: pullulanase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.54Å 60.66Å 135.39Å 90.00° 113.59° 90.00°	Depositor
Resolution (Å)	14.99 – 1.85 47.89 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.9 (14.99-1.85) 90.7 (47.89-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.214 0.178 , 0.214	Depositor DCC
R_{free} test set	8791 reflections (11.11%)	DCC
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 94287 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9357	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/8387	0.58	0/11418

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8142	0	7841	211	0
2	A	68	0	60	2	0
3	A	23	0	21	0	0
4	A	5	0	0	0	0
5	A	1119	0	0	14	0
All	All	9357	0	7922	211	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (211) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:81:ASN:HB2	1:A:86:ASP:HA	1.44	0.98
1:A:978:ASN:HD21	1:A:984:GLN:H	1.16	0.92
1:A:40:VAL:HG13	1:A:41:ALA:H	1.38	0.89
1:A:81:ASN:HD22	1:A:88:LEU:HB2	1.38	0.89
1:A:83:GLU:HG3	1:A:84:THR:H	1.39	0.88
1:A:680:LEU:HD11	5:A:1543:HOH:O	1.78	0.84
1:A:127:VAL:HG21	1:A:153:VAL:HG21	1.59	0.82
1:A:972[A]:LYS:HE2	1:A:973:ARG:HE	1.47	0.80
1:A:606:ASN:HD21	1:A:607:HIS:HD2	1.31	0.79
1:A:452[A]:LEU:HD12	1:A:587:MET:HG3	1.64	0.78
1:A:229:ASN:HD21	1:A:232:VAL:CG2	1.99	0.76
1:A:229:ASN:HD21	1:A:232:VAL:HG23	1.50	0.76
1:A:972[A]:LYS:HG3	1:A:973:ARG:HG3	1.69	0.75
1:A:184:LYS:HD2	1:A:185:THR:H	1.50	0.75
1:A:79:LEU:HB3	1:A:88:LEU:HD13	1.70	0.74
1:A:722:ILE:HD12	5:A:2376:HOH:O	1.87	0.74
1:A:82:ASN:ND2	1:A:83:GLU:HG2	2.02	0.73
1:A:37:LEU:HD13	1:A:169:ARG:HB3	1.73	0.71
1:A:76:ASN:ND2	1:A:128:ARG:HH21	1.90	0.69
1:A:219:LYS:HD3	1:A:219:LYS:H	1.58	0.69
1:A:560:ASP:HB3	1:A:609:ASN:ND2	2.09	0.68
1:A:680:LEU:HG	1:A:710:SER:HB3	1.76	0.67
1:A:606:ASN:ND2	1:A:607:HIS:HD2	1.90	0.67
1:A:523:THR:OG1	1:A:526:GLU:HG3	1.93	0.67
1:A:184:LYS:HD2	1:A:185:THR:N	2.10	0.66
1:A:501:ARG:O	1:A:504:GLU:HG2	1.96	0.66
1:A:50:SER:H	1:A:53:GLN:NE2	1.94	0.66
1:A:82:ASN:HD22	1:A:83:GLU:HG2	1.60	0.66
1:A:627:TYR:O	1:A:651:HIS:HD2	1.79	0.66
1:A:40:VAL:HG13	1:A:41:ALA:N	2.10	0.65
1:A:972[A]:LYS:HE2	1:A:973:ARG:NE	2.11	0.65
1:A:76:ASN:HD21	1:A:128:ARG:HH21	1.45	0.65
1:A:1049:GLN:HG3	1:A:1057:THR:HB	1.78	0.65
1:A:680:LEU:HD13	1:A:708:TRP:HB2	1.80	0.64
1:A:61:ILE:O	1:A:64:ILE:HG12	1.98	0.63
1:A:1028:THR:O	1:A:1029:SER:HB3	1.99	0.63
1:A:411[A]:MET:HE3	5:A:2250:HOH:O	1.99	0.62
1:A:680:LEU:HD23	1:A:680:LEU:H	1.65	0.62
1:A:560:ASP:HB3	1:A:609:ASN:HD22	1.64	0.62
1:A:40:VAL:HG22	1:A:41:ALA:N	2.15	0.62
1:A:184:LYS:HD3	1:A:185:THR:HG23	1.80	0.61
1:A:324:SER:HB3	1:A:330[A]:ILE:HD11	1.81	0.61
1:A:75:LYS:O	1:A:102:PRO:HD3	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:78:TYR:HB3	1:A:126:ILE:HB	1.83	0.60
1:A:123:ILE:HD11	1:A:141:VAL:HB	1.83	0.60
1:A:193:GLU:O	1:A:194:ASN:HB2	2.00	0.60
1:A:81:ASN:CB	1:A:86:ASP:HA	2.28	0.59
1:A:987:LEU:HD21	1:A:1022:LEU:HD21	1.84	0.59
1:A:465:GLN:HG3	1:A:950:GLN:HE22	1.67	0.58
1:A:452[A]:LEU:HD12	1:A:587:MET:CG	2.32	0.58
1:A:87:ALA:HB3	1:A:123:ILE:HG23	1.84	0.58
1:A:55:VAL:HG23	1:A:150:THR:HG23	1.85	0.58
1:A:969:THR:HA	1:A:972[A]:LYS:HG2	1.85	0.58
1:A:123:ILE:HD12	1:A:123:ILE:O	2.04	0.57
1:A:197:ILE:HD12	1:A:270:GLY:HA2	1.86	0.57
1:A:706:GLU:OE2	2:A:1098:GLC:H1	2.05	0.57
1:A:80:TRP:CZ3	1:A:126:ILE:HG13	2.40	0.57
1:A:79:LEU:O	1:A:92:VAL:HG22	2.04	0.57
1:A:680:LEU:N	1:A:680:LEU:HD23	2.19	0.57
1:A:50:SER:H	1:A:53:GLN:HE21	1.52	0.56
1:A:682:HIS:HD2	1:A:686:GLN:NE2	2.03	0.56
1:A:80:TRP:HZ3	1:A:126:ILE:HG13	1.69	0.56
1:A:246:LYS:HD3	1:A:247:LEU:N	2.21	0.56
1:A:95:TRP:HH2	1:A:133:LYS:HG2	1.71	0.55
1:A:1039:ALA:HB3	1:A:1043:SER:HB2	1.88	0.55
1:A:139:LEU:H	1:A:139:LEU:HD12	1.70	0.55
1:A:85:CYS:HB3	1:A:122:CYS:O	2.07	0.55
1:A:195:LYS:N	1:A:195:LYS:HE3	2.21	0.55
1:A:682:HIS:HD2	1:A:686:GLN:HE22	1.54	0.55
1:A:816:PRO:HG2	5:A:1995:HOH:O	2.07	0.55
1:A:107:LYS:HD2	1:A:107:LYS:H	1.71	0.55
1:A:229:ASN:HD21	1:A:232:VAL:CB	2.20	0.54
1:A:929:ARG:HD2	5:A:1588:HOH:O	2.07	0.54
1:A:76:ASN:HD21	1:A:128:ARG:NH2	2.06	0.54
1:A:229:ASN:N	1:A:229:ASN:HD22	2.06	0.53
1:A:642:THR:O	1:A:643:CYS:HB3	2.08	0.53
1:A:977:ARG:NH1	1:A:1024:ASP:HB3	2.24	0.53
1:A:496:GLN:H	1:A:496:GLN:NE2	2.06	0.53
1:A:495:ILE:HA	1:A:524:VAL:HB	1.91	0.53
1:A:81:ASN:HB2	1:A:86:ASP:CA	2.30	0.53
1:A:98:VAL:HG22	1:A:98:VAL:O	2.09	0.52
1:A:81:ASN:HD21	1:A:91:PRO:HD3	1.74	0.52
1:A:418:LYS:HD2	1:A:966[A]:ASP:OD1	2.09	0.52
1:A:55:VAL:CG2	1:A:150:THR:HG23	2.40	0.52
1:A:65:THR:HG23	1:A:66:SER:H	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:680:LEU:CD2	1:A:680:LEU:H	2.22	0.52
1:A:122:CYS:HB3	1:A:142:SER:HA	1.92	0.52
1:A:977:ARG:HH11	1:A:1024:ASP:HB3	1.75	0.52
1:A:969:THR:HG23	1:A:972[A]:LYS:NZ	2.25	0.52
1:A:387:ASN:ND2	1:A:487:GLU:H	2.08	0.52
1:A:65:THR:HG23	1:A:66:SER:N	2.25	0.51
1:A:36:ARG:HB3	1:A:215:GLU:HA	1.91	0.51
1:A:208:VAL:HG22	1:A:260:GLU:OE2	2.11	0.51
1:A:56:ILE:HD11	1:A:153:VAL:HG13	1.92	0.51
1:A:452[A]:LEU:HD13	1:A:591:ILE:HD11	1.93	0.50
1:A:56:ILE:HD13	1:A:151:VAL:HG23	1.93	0.50
1:A:946:THR:O	1:A:950:GLN:HG3	2.11	0.50
1:A:272:LEU:C	1:A:272:LEU:HD23	2.31	0.50
1:A:60:ASP:OD2	1:A:62:ALA:HB3	2.12	0.50
1:A:229:ASN:ND2	1:A:232:VAL:HB	2.27	0.50
1:A:49:ALA:HB1	1:A:53:GLN:O	2.12	0.50
1:A:745:PRO:HG2	1:A:746:PHE:CE1	2.46	0.50
1:A:38:PRO:HG3	1:A:271:ILE:HD11	1.93	0.49
1:A:33:VAL:HG21	1:A:197:ILE:CD1	2.42	0.49
1:A:682:HIS:CD2	1:A:686:GLN:HE22	2.31	0.49
1:A:466:LEU:HD23	1:A:950:GLN:HE21	1.76	0.49
1:A:324:SER:HB3	1:A:330[B]:ILE:HD11	1.95	0.49
1:A:198:VAL:HG12	1:A:223:LEU:HD12	1.95	0.49
1:A:55:VAL:HA	1:A:112:TRP:O	2.12	0.49
1:A:87:ALA:HB3	1:A:123:ILE:CG2	2.43	0.48
1:A:128:ARG:HA	1:A:134:LEU:H	1.77	0.48
1:A:1049:GLN:CG	1:A:1057:THR:HB	2.43	0.48
1:A:80:TRP:CZ2	1:A:124:ASN:HB3	2.48	0.48
1:A:678:LEU:C	1:A:680:LEU:HD23	2.33	0.48
1:A:465:GLN:HG3	1:A:950:GLN:NE2	2.28	0.48
1:A:134:LEU:HD22	1:A:155:ALA:HA	1.95	0.48
1:A:154:ILE:HD11	1:A:167:ALA:HB1	1.94	0.48
1:A:38:PRO:HA	1:A:271:ILE:HD11	1.95	0.48
1:A:267:GLU:HB2	1:A:271:ILE:HG22	1.95	0.48
1:A:184:LYS:HG3	1:A:286:ASP:OD2	2.13	0.48
1:A:39:ASP:HA	1:A:42:VAL:HG21	1.95	0.48
1:A:465:GLN:CG	1:A:950:GLN:HE22	2.27	0.48
1:A:643:CYS:SG	1:A:644:CYS:N	2.87	0.48
1:A:58:LEU:CD2	1:A:75:LYS:HD3	2.44	0.47
1:A:77:LEU:CD2	1:A:127:VAL:HA	2.44	0.47
1:A:125:VAL:HG12	1:A:126:ILE:N	2.29	0.47
1:A:139:LEU:N	1:A:139:LEU:HD12	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:TRP:O	1:A:124:ASN:HB2	2.15	0.47
1:A:230:GLN:O	1:A:234:MET:HG2	2.15	0.47
1:A:461[B]:GLN:NE2	5:A:1950:HOH:O	2.47	0.47
1:A:606:ASN:ND2	1:A:607:HIS:CD2	2.77	0.47
1:A:46:ALA:HB3	1:A:57:HIS:CE1	2.50	0.47
1:A:411[B]:MET:HE3	5:A:1702:HOH:O	2.14	0.46
1:A:139:LEU:H	1:A:139:LEU:CD1	2.28	0.46
1:A:642:THR:O	1:A:643:CYS:CB	2.63	0.46
1:A:154:ILE:HG22	1:A:155:ALA:N	2.31	0.46
1:A:246:LYS:HD3	1:A:247:LEU:O	2.15	0.46
1:A:85:CYS:HB3	1:A:122:CYS:C	2.35	0.46
1:A:693[B]:ARG:NH2	5:A:1547:HOH:O	2.49	0.46
1:A:302:THR:HG23	5:A:1944:HOH:O	2.15	0.46
1:A:430:HIS:HD2	1:A:433:ASP:H	1.62	0.46
1:A:231:GLN:N	1:A:231:GLN:OE1	2.49	0.46
1:A:79:LEU:CD2	1:A:125:VAL:HG22	2.45	0.46
1:A:197:ILE:HB	1:A:266:ALA:HB3	1.98	0.46
1:A:123:ILE:HD13	1:A:125:VAL:HG23	1.97	0.46
1:A:199:ARG:HD3	1:A:220:TYR:CE2	2.51	0.46
1:A:154:ILE:HD11	1:A:167:ALA:O	2.15	0.46
1:A:38:PRO:CA	1:A:271:ILE:HD11	2.46	0.45
1:A:219:LYS:HD3	1:A:219:LYS:N	2.28	0.45
1:A:592:LYS:HE2	1:A:672:ASP:OD2	2.16	0.45
1:A:1028:THR:O	1:A:1029:SER:CB	2.64	0.45
1:A:680:LEU:HD12	1:A:710:SER:N	2.32	0.45
1:A:98:VAL:HG12	5:A:2386:HOH:O	2.15	0.45
1:A:195:LYS:HE3	1:A:195:LYS:CA	2.47	0.45
1:A:56:ILE:CG2	1:A:112:TRP:HB2	2.47	0.45
1:A:123:ILE:CD1	1:A:141:VAL:HB	2.46	0.45
1:A:229:ASN:HD21	1:A:232:VAL:HB	1.81	0.45
1:A:430:HIS:CD2	1:A:432:ARG:H	2.35	0.45
1:A:886:SER:O	1:A:887:PHE:HB2	2.17	0.44
1:A:94:ASP:OD2	1:A:96:ASN:HB2	2.18	0.44
1:A:229:ASN:N	1:A:229:ASN:ND2	2.66	0.44
1:A:68:THR:OG1	1:A:69:PRO:HD2	2.18	0.44
1:A:1014:ASN:HD21	1:A:1020:ARG:HH11	1.65	0.44
1:A:81:ASN:HD22	1:A:88:LEU:CB	2.19	0.43
1:A:33:VAL:HG21	1:A:197:ILE:HD13	1.99	0.43
1:A:210:ALA:HA	1:A:215:GLU:O	2.17	0.43
1:A:366:PRO:HB2	1:A:626:TRP:CE2	2.52	0.43
1:A:750:ASP:HB3	1:A:754:GLN:HE21	1.83	0.43
1:A:677:ASP:OD1	2:A:1098:GLC:H1	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:LYS:HD2	1:A:107:LYS:N	2.34	0.43
1:A:204:HIS:HE1	5:A:1154:HOH:O	2.00	0.43
1:A:228:VAL:O	1:A:228:VAL:HG13	2.18	0.43
1:A:680:LEU:HD12	1:A:709:ASP:C	2.38	0.43
1:A:56:ILE:HG21	1:A:77:LEU:CD1	2.49	0.43
1:A:100:THR:HG22	1:A:100:THR:O	2.17	0.43
1:A:77:LEU:HD23	1:A:127:VAL:HA	2.00	0.43
1:A:773:SER:OG	1:A:776:GLN:HG3	2.19	0.43
1:A:57:HIS:HB2	1:A:152:SER:OG	2.18	0.43
1:A:510:LYS:HE2	5:A:1189:HOH:O	2.19	0.42
1:A:238:HIS:H	1:A:238:HIS:CD2	2.37	0.42
1:A:40:VAL:CG1	1:A:41:ALA:N	2.78	0.42
1:A:430:HIS:HB3	1:A:433:ASP:HB2	2.00	0.42
1:A:123:ILE:HD12	1:A:123:ILE:C	2.40	0.42
1:A:260:GLU:HB2	1:A:364:TYR:CE1	2.55	0.42
1:A:486:ASN:HB2	5:A:1693:HOH:O	2.19	0.42
1:A:722:ILE:HG13	5:A:1665:HOH:O	2.20	0.42
1:A:47:VAL:HG22	1:A:48:GLN:N	2.35	0.42
1:A:36:ARG:HB2	1:A:214:GLY:O	2.20	0.42
1:A:39:ASP:HA	1:A:42:VAL:CG2	2.50	0.42
1:A:216:PHE:CZ	1:A:272:LEU:HD13	2.55	0.41
1:A:494:ASP:HB3	1:A:496:GLN:HE22	1.84	0.41
1:A:948:PHE:CD1	1:A:1044:LEU:HG	2.55	0.41
1:A:83:GLU:HG3	1:A:84:THR:N	2.19	0.41
1:A:56:ILE:HG21	1:A:77:LEU:HD11	2.03	0.41
1:A:187:LEU:C	1:A:187:LEU:HD13	2.41	0.41
1:A:734:ASP:OD1	1:A:734:ASP:N	2.53	0.41
1:A:199:ARG:HB2	1:A:201:TYR:HE1	1.85	0.41
1:A:203:SER:OG	1:A:206:SER:HB2	2.19	0.41
1:A:128:ARG:HA	1:A:134:LEU:HB2	2.03	0.41
1:A:126:ILE:HD11	1:A:138:ASP:OD1	2.21	0.41
1:A:197:ILE:O	1:A:265:ALA:HA	2.21	0.41
1:A:136:ASP:O	1:A:137:SER:HB2	2.20	0.40
1:A:680:LEU:CG	1:A:710:SER:HB3	2.49	0.40
1:A:746:PHE:N	1:A:746:PHE:CD1	2.88	0.40
1:A:682:HIS:CD2	1:A:686:GLN:NE2	2.87	0.40
1:A:183:ASP:OD2	1:A:186:THR:N	2.54	0.40
1:A:149:ARG:HG3	1:A:149:ARG:HH11	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1070/1083 (99%)	1008 (94%)	52 (5%)	10 (1%)	25 8

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	66	SER
1	A	83	GLU
1	A	218	ASP
1	A	93	ALA
1	A	478	PRO
1	A	643	CYS
1	A	1029	SER
1	A	209	ALA
1	A	91	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	886/891 (99%)	869 (98%)	17 (2%)	69 55

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	LYS
1	A	184	LYS
1	A	195	LYS
1	A	229	ASN

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Mol	Chain	Res	Type
1	A	252	ASN
1	A	374	TYR
1	A	387	ASN
1	A	478	PRO
1	A	482	LEU
1	A	496	GLN
1	A	543	GLN
1	A	562	PHE
1	A	746	PHE
1	A	831	SER
1	A	859	GLN
1	A	886	SER
1	A	1049	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	53	GLN
1	A	76	ASN
1	A	81	ASN
1	A	204	HIS
1	A	213	ASN
1	A	229	ASN
1	A	230	GLN
1	A	238	HIS
1	A	252	ASN
1	A	279	GLN
1	A	316	GLN
1	A	387	ASN
1	A	392	GLN
1	A	413	HIS
1	A	430	HIS
1	A	439	GLN
1	A	455	GLN
1	A	458	ASN
1	A	465	GLN
1	A	496	GLN
1	A	533	GLN
1	A	534	ASN
1	A	541	GLN
1	A	543	GLN

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Mol	Chain	Res	Type
1	A	551	GLN
1	A	563	HIS
1	A	606	ASN
1	A	607	HIS
1	A	609	ASN
1	A	651	HIS
1	A	682	HIS
1	A	686	GLN
1	A	754	GLN
1	A	835	ASN
1	A	859	GLN
1	A	899	ASN
1	A	911	ASN
1	A	950	GLN
1	A	978	ASN
1	A	983	GLN
1	A	1014	ASN
1	A	1023	GLN
1	A	1037	GLN
1	A	1074	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	A	1092	2	10,11,12	0.42	0	11,15,17	0.21	0
2	GLC	A	1093	2	10,11,12	0.39	0	11,15,17	0.36	0
2	GLC	A	1094	2	12,12,12	0.44	0	17,17,17	0.40	0
2	GLC	A	1096	2	10,11,12	0.39	0	11,15,17	0.26	0
2	GLC	A	1097	2	10,11,12	0.43	0	11,15,17	0.39	0
2	GLC	A	1098	2	12,12,12	0.47	0	17,17,17	0.67	0
3	GLC	A	1099	3	10,11,12	0.39	0	11,15,17	0.28	0
3	GLC	A	1100	3	12,12,12	0.39	0	17,17,17	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	1092	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1093	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1094	2	-	0/2/22/22	0/1/1/1
2	GLC	A	1096	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1097	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1098	2	-	0/2/22/22	0/1/1/1
3	GLC	A	1099	3	-	0/2/19/22	0/1/1/1
3	GLC	A	1100	3	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1052/1083 (97%)	0.36	129 (12%) 5 5	11, 20, 73, 85	124 (11%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	VAL	11.7
1	A	90	ALA	8.7
1	A	122	CYS	8.2
1	A	84	THR	8.1
1	A	88	LEU	8.0
1	A	64	ILE	7.7
1	A	80	TRP	7.5
1	A	79	LEU	7.5
1	A	81	ASN	7.3
1	A	142	SER	7.3
1	A	91	PRO	7.2
1	A	133	LYS	7.1
1	A	39	ASP	6.8
1	A	62	ALA	6.8
1	A	82	ASN	6.8
1	A	40	VAL	6.7
1	A	54	ALA	6.6
1	A	123	ILE	6.4
1	A	87	ALA	6.4
1	A	93	ALA	6.4
1	A	271	ILE	6.3
1	A	139	LEU	6.3
1	A	98	VAL	6.1
1	A	160	VAL	6.1
1	A	143	PHE	6.0
1	A	129	ASP	6.0
1	A	86	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	141	VAL	5.8
1	A	127	VAL	5.7
1	A	272	LEU	5.6
1	A	154	ILE	5.5
1	A	117	THR	5.3
1	A	38	PRO	5.3
1	A	56	ILE	5.2
1	A	95	TRP	5.2
1	A	128	ARG	5.2
1	A	169	ARG	5.2
1	A	116	LEU	5.2
1	A	216	PHE	5.1
1	A	59	VAL	5.1
1	A	131	THR	4.9
1	A	212	SER	4.9
1	A	136	ASP	4.9
1	A	61	ILE	4.8
1	A	41	ALA	4.7
1	A	167	ALA	4.7
1	A	270	GLY	4.6
1	A	196	PRO	4.6
1	A	76	ASN	4.5
1	A	158	SER	4.5
1	A	94	ASP	4.4
1	A	135	ILE	4.4
1	A	168	PHE	4.4
1	A	161	TYR	4.4
1	A	144	SER	4.3
1	A	166	ASP	4.3
1	A	125	VAL	4.2
1	A	159	ALA	4.0
1	A	217	SER	4.0
1	A	157	ASN	3.9
1	A	170	ALA	3.9
1	A	137	SER	3.9
1	A	130	GLY	3.8
1	A	89	SER	3.8
1	A	195	LYS	3.8
1	A	74	THR	3.7
1	A	210	ALA	3.7
1	A	145	ASP	3.7
1	A	140	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	194	ASN	3.6
1	A	35	VAL	3.6
1	A	63	GLY	3.5
1	A	197	ILE	3.5
1	A	55	VAL	3.5
1	A	213	ASN	3.5
1	A	85	CYS	3.4
1	A	65	THR	3.4
1	A	83	GLU	3.4
1	A	303	ASP	3.3
1	A	146	PHE	3.3
1	A	60	ASP	3.3
1	A	42	VAL	3.2
1	A	33	VAL	3.2
1	A	1027	GLY	3.2
1	A	34	VAL	3.1
1	A	67	SER	3.1
1	A	37	LEU	3.1
1	A	268	SER	3.1
1	A	172	PHE	3.1
1	A	147	THR	3.0
1	A	265	ALA	3.0
1	A	134	LEU	2.9
1	A	69	PRO	2.9
1	A	247	LEU	2.9
1	A	138	ASP	2.9
1	A	209	ALA	2.9
1	A	198	VAL	2.7
1	A	97	ASP	2.7
1	A	151	VAL	2.7
1	A	201	TYR	2.6
1	A	174	VAL	2.6
1	A	162	ASP	2.6
1	A	78	TYR	2.6
1	A	66	SER	2.6
1	A	211	ASP	2.5
1	A	242	TYR	2.5
1	A	114	ILE	2.5
1	A	269	ASP	2.5
1	A	156	GLY	2.5
1	A	132	ASN	2.5
1	A	32	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	36	ARG	2.4
1	A	266	ALA	2.4
1	A	153	VAL	2.4
1	A	746	PHE	2.4
1	A	58	LEU	2.4
1	A	165	ALA	2.4
1	A	192	GLY	2.3
1	A	112	TRP	2.2
1	A	246	LYS	2.2
1	A	214	GLY	2.2
1	A	52	ARG	2.2
1	A	250	ASP	2.2
1	A	110	PRO	2.1
1	A	155	ALA	2.1
1	A	208	VAL	2.1
1	A	176	LEU	2.1
1	A	249	ASP	2.0
1	A	150	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GLC	A	1099	11/12	0.41	1.29	87,88,88,88	0
2	GLC	A	1096	11/12	0.09	0.60	21,24,28,31	0
3	GLC	A	1100	12/12	0.42	0.48	88,88,88,88	0
2	GLC	A	1097	11/12	0.09	0.18	13,17,18,18	0
2	GLC	A	1098	12/12	0.11	-0.18	17,21,23,27	0
2	GLC	A	1093	11/12	0.09	-0.62	21,22,27,36	0
2	GLC	A	1092	11/12	0.08	-0.74	21,23,26,27	0
2	GLC	A	1094	12/12	0.08	-0.89	18,19,21,25	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CA	A	2402	1/1	0.12	0.74	34,34,34,34	0
4	CA	A	2401	1/1	0.07	-0.09	16,16,16,16	0
4	CA	A	2404	1/1	0.06	-1.22	16,16,16,16	0
4	CA	A	2403	1/1	0.06	-1.27	36,36,36,36	0
4	CA	A	2405	1/1	0.11	-1.89	59,59,59,59	0

6.5 Other polymers

There are no such residues in this entry.